

FRUSTRATED SPIN SYSTEMS

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ABSTRACT — This paper aims to review mostly rigorous results on frustrated Ising systems and present a unified approach to the statistical mechanics of frustrated systems. The formalism is presented in a general enough manner to include q -state Potts models wherever this extension was possible.

I — INTRODUCTION

The present review was motivated by two lectures I gave at the Laboratorio de Física, Faculdade de Ciências, in Porto. It is intended as a tutorial introduction to the subject, with a pedestrian's approach to the connection with gauge theories. The interested reader is encouraged to go to other existing reviews in the field, notably that by Toulouse (1980), and to the seminal article of Fradkin et al. (1978).

Although in this review I will confine myself to spin models, the usefulness of the concept of frustration is certainly not limited to spin models. The ideas of frustrations and frustration lines have been extended by various authors to continuum models (see for example Dzyaloshinskii and Volovik 1980, and the review article by Halperin 1981 as well as the more recent work of Rivier).

I have, moreover, both for the sake of brevity and unity of presentation, not included models with continuous symmetries, although a few references have found their way in. (This is a big

shortcoming, as some of the most interesting results, analogies and open questions are to be found precisely in these systems). Above all, I do not pretend to make an exhaustive review of the subject, but hope to have included the highlights of the progress in the field, enough to indicate problems and loose ends. At the same time I hope I have been able to introduce the reader to some useful techniques in dealing with frustrated systems.

The paper is organized as follows. In Section II, I will give an intuitive definition of frustration and then proceed to review the results on ground state properties, the existence or nonexistence of phase transitions and their universality class, and the behaviour of the correlation functions, in periodically frustrated and, where available, on randomly frustrated Ising models. (The fully frustrated (ff) models are a special case of the former). This is not meant to be a review of the vast literature existing on spin glasses (SG), and only a few papers dealing with randomly frustrated systems are touched upon, the selection having been made on the basis of emphasis, namely, on the direct interrelation between the behaviour of the system and that of the distribution of frustrations.

In Section III, I introduce the concept of gauge variables and gauge transformations. The invariance of the partition function under these transformations is derived. The continuity between annealed and quenched averages is demonstrated.

In Section IV, the duality transformation and disorder variables are introduced. The interrelations under duality transformations, between disorder-disorder correlation functions in two dimensions (2d) (gauge invariant correlation functions in three dimensions (3d)) and the defects in the ordered spin system are displayed. The relevance of these correlation functions to the probability distributions of configurations of frustrations (and thus quenched averages) is shown. Finally, phase transitions in the frustration system as a function of the concentration of antiferromagnetic (AFM) or ferromagnetic (FM) bonds are considered.

Where possible, the material in Sections III and IV has been presented with enough generality to cover systems with Z_N type symmetries, and some consequences of the generalization to Potts systems of analogous results on the Ising model are indicated.

II — FRUSTRATED SYSTEMS

Consider a system of spin s_i located on the sites, i , of a lattice, with interactions J_{ij} on the bonds. The Hamiltonian is given by

$$H = - \sum_{(ij)} J_{ij} f(s_i, s_j) = \sum_{(ij)} E_{ij} \quad (2.1)$$

where the sum is over all pairs i, j . The most intuitive definition of frustration is to say that the system is *frustrated*, if not all E_{ij} may take their minimum values simultaneously, for any configuration of the spins s_i . Observe that this is a property of the set of interactions J_{ij} on the bonds and the functions $f(s_i, s_j)$; however it does not depend on a particular set of values of the functions $f(s_i, s_j)$ or s_i . From now on we will refer to the situation where E_{ij} takes its minimum value as 'the bond (i, j) being *satisfied*'. (Otherwise, we shall say it is *broken*. Using 'frustrated' in this context gives rise to a lot of confusion).

Let us illustrate. The simplest such spin model is the Ising model, where

$$s_i = \pm 1; \quad f(s_i, s_j) = s_i s_j \quad (2.2)$$

It is obvious that on a one dimensional chain with only nearest neighbor interactions (no overlapping bonds) and open ends, it is always possible for the s_i to take on a set of values which will satisfy any given set of J_{ij} . However, as soon as we have a closed loop of bonds, e.g. a triangle with the set J_{ij} of bonds on the edges as shown in Fig. 1a, b the problem is no longer trivial. In fact both of these systems are *frustrated*. It can easily be checked that any such loop with an odd number of bonds equal to $-J$, and the rest equal to J , is frustrated. Moreover, any lattice in d dimensions, incorporating such loops will also be frustrated.

Toulouse (1977) has defined the *frustration function* for the Ising model to be given by

$$\phi_p = \text{sgn} \left(\prod_p J_{ij} \right) \quad (2.3)$$

where the product is over all the bonds on a loop p . This function is positive if the loop is not frustrated, and negative if it is. If this

loop is the smallest loop that can be constructed on the given lattice, it will be called a plaquette. If the function ϕ_p associated with some plaquette is negative, that plaquette will be said to be frustrated, or is a 'frustration'.

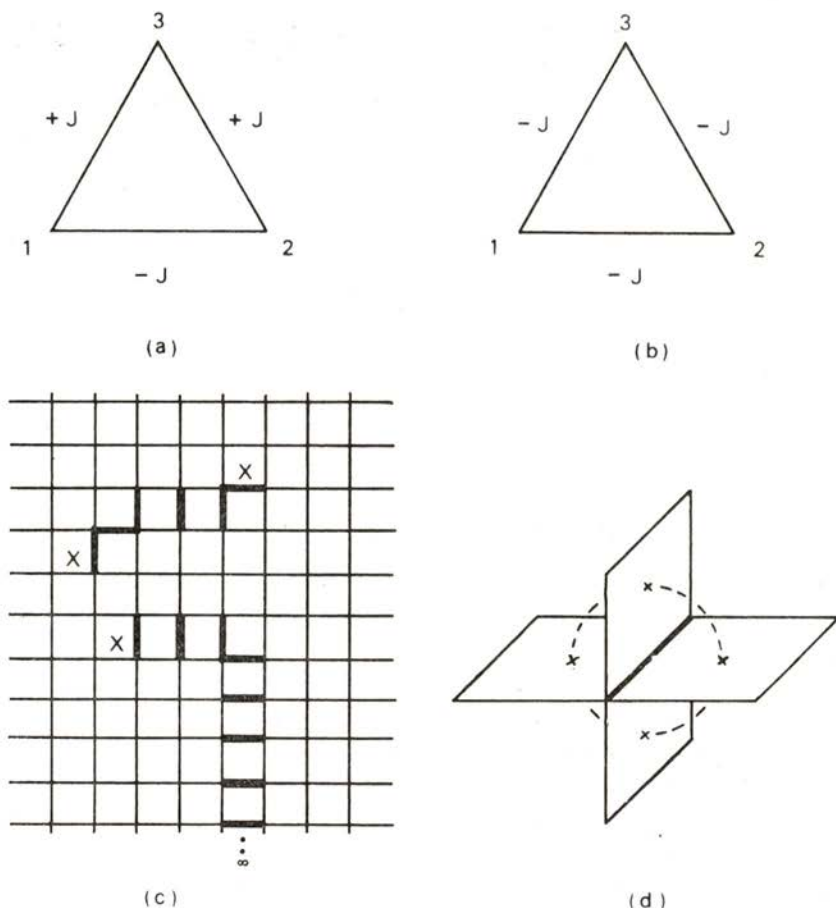


Fig. 1 — (a), (b) Simple frustrated plaquettes, (c) possible configurations of frustrations in two dimensions, (d) smallest possible 'tube' of frustrations in three dimensions. Dark lines are AFM. Frustrations are marked with an 'x'.

The distribution of frustrations on a lattice in d dimensions obeys certain topological constraints. As can be seen from Fig. 1c,

in two dimensions, any finite number of AFM bonds give rise only to pairs of frustrations. A single frustration can only be created with an infinite 'ladder' of AFM bonds going out to the edge of the lattice. In three dimensions, only a closed 'tube' of frustrated plaquettes may exist, the smallest possible such 'tube', surrounding a single AFM bond is shown in Fig. 1d (Fradkin et al. 1978). One can see that in the ordered phase spins would tend to align parallel, except along the faults, or defects, created by the AFM bonds, with the frustrations in two dimensions acting as the sources and sinks of the defect line. In three dimensions, an arbitrary loop of frustrated plaquettes is created by flipping all the spins incident on some surface bounded by this loop.

The concept of frustration has been generalized to other types of spin systems. The frustrated $x-y$ model has been treated by Villain (1977b), Fradkin et al. (1978), José (1979), and more recently by Dzyaloshinskii and Obukov (1982). The latter have also treated a frustrated Heisenberg model. The extension to continuous spins has been provided by Herz (1978). In this review, I will, as already stated, stay for the most part with the Ising model. In section III, and IV, a more general treatment will also include the Potts model.

The usefulness of this quantity can be illustrated as follows: There are many conceivable ways in which bond randomness may be introduced into a Hamiltonian like Eq. (2.1), allowing for J_{ij} to take on both positive and negative values. (For simplicity, let us for the moment assume that the magnitude of the coupling constant stays the same). However it turns out that the models obtained via some of these schemes may be transformed, by a suitable redefinition of the spins, into uniform ferromagnetic models, and thus contain a 'hidden order parameter', namely the magnetization of the related ferromagnetic model. The partition functions and the free energies of the original and transformed models are of course the same, and so are the singularities encountered at the transition temperature, if there is one. The classical example of this phenomenon is the 'Mattis model' (Mattis 1976), where

$$J_{ij} = J \sigma_i \sigma_j \quad , \quad \sigma_i = \pm 1$$

and σ_i, σ_j are independent random variables. For Ising spin s_i one may define

$$\tau_i = s_i \sigma_i$$

so that the partition function

$$Z = \sum_{\{s_i\}} \exp \left[\beta J \sum_{(ij)} \sigma_i \sigma_j s_i s_j \right]$$

reduces identically to that of the ferromagnetic Ising model:

$$Z = \sum_{\{\tau_i\}} \exp \left[\beta J \sum_{(ij)} \tau_i \tau_j \right]$$

where β is the inverse temperature in units of the Boltzmann constant, as usual. Note that although $\langle s_i \rangle = 0$ for all temperatures, for an even distribution of the σ_i , $\langle \tau_i \rangle > 0$ for $T < T_c$, where T_c is the critical temperature of the ferromagnetic model. (See Section III for a more general discussion of this type of transformation). Upon inspecting the original model we see that it is completely unfrustrated! For any closed loop on the lattice,

$$\prod_c \sigma_i \sigma_j \equiv 1$$

where the product is over all pairs i, j lying on the loop c . An inspection of the ground state of the system will show that there is in fact a unique way (with the overall degeneracy of 2) of choosing the spins s_i such that all the bonds $J_{ij} = J \sigma_i \sigma_j$ are satisfied. This ground state is precisely the ferromagnetic ground state in the variables τ_i . In section III we will see that a system with frustrations cannot be transformed into an unfrustrated system by such a redefinition of the spins. We conclude that frustration is a *necessary and irreducible* feature of spin glass models.

Random and Periodically Frustrated Systems

An Ising spin glass model where the exchange interactions are distributed independently of each other with some probability $P(J)$, where $P(J)$ includes negative couplings, will give rise

to a lattice with a random distribution of frustrations. (In fact, on a square lattice with an even distribution of $+$, $-$ bonds, exactly half the plaquettes will be frustrated on the average). One may, on the other hand, construct periodic arrays of frustrated plaquettes, or systems where each plaquette is frustrated, namely, *fully frustrated* systems. (See Fig. 2 for the fully frustrated

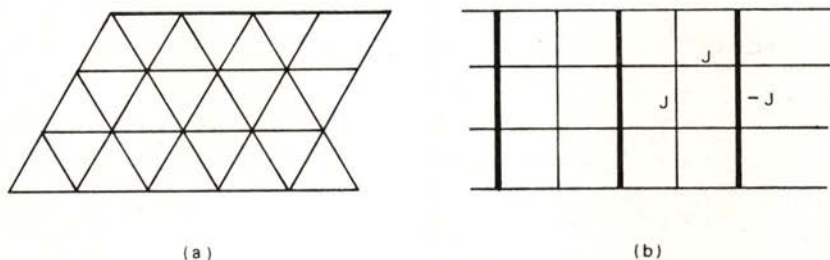


Fig. 2 — (a) Segment of the triangular lattice. Fully frustrated with all AFM interactions, this lattice corresponds to the fcc lattice in three dimensions, and generalizations thereof in higher dimensionality. (Alexander and Pincus 1980). (b) The Odd Model (FFSI) in two dimensions. This model can also be generalized to the fully frustrated hypercubic lattice in d dimensions. (Derrida et al. 1979, Villain 1977 a).

lattices to which we will most frequently refer). Since the periodic systems are easier to treat, and in fact in two dimensions can be solved exactly (Ising, Potts) a lot of effort has gone into determining their properties. (See Fig. 3 and the references given there). Moreover, by considering periodic strips in 2-d, within each of which the distribution of frustrated layers might be random, and then letting the width of these strips go to infinity, certain results may be obtained on systems with translational invariance in one direction and complete randomness on the other. (Hoever et al. 1981, Kardar and Berker 1982). I shall try to review these results here from the point of view of ground state properties, the existence or nonexistence of a phase transition, the nature of the low temperature or zero temperature phase and the behaviour of the correlation functions.

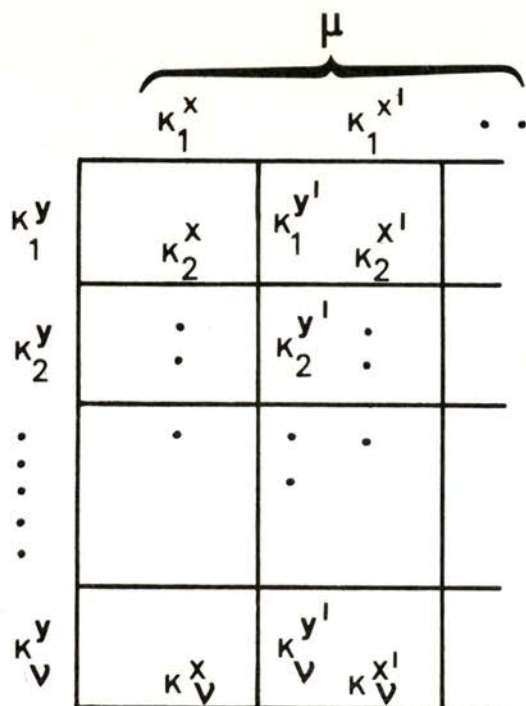


Fig. 3—Periodically frustrated lattices. For $\mu = 1$, n = number of AFM rows and m = number of FM rows in ν .

- (a) $\mu = 1$. Hoever and Zittartz (1981), Wolff et al. (1981).
- (b) $\mu = 1$. Kardar and Berker (1982).
- (c) $\mu = 1$, $|K_1^y| = \text{constant}$. Hoever et al. (1981), where the same frustration distribution with the minimum number of AFM bonds is also considered. Hoever et al. (1981), Bryskin et al. (1980) with $n = 1$, $m = 3$.
- (d) $\mu = 1$, $\nu = 1, 2, 3$, $n/m = 1, 1/2, 1/3$. Longa and Olés (1980).
- (e) $\mu = 1$, $\nu = 2$, $|K^y| = |K^x|$ (DUD), $\mu = 2$; $\nu = 2$, $J = K_1^y = K_2^y$, $K_2^y = K_1^{y'} = J'$ (ZZD). André et al. (1979).
- (f) $\mu = 2$, $\nu = 2$, $K_1^x = K_2^{x'} = J_2$, $K_1^{x'} = K_2^x = J_4$, $K_1^y = K_2^{y'} = J_3$, $K_2^y = K_1^{y'} = J_1$. Gabay (1980).
- (g) $\mu = 2$, $\nu = 2$, $K_1^{y'} = -K_1^y = J_2$, $K_2^{y'} = -K_2^y = J_4$, $K_2^x = K_1^x = J_3$, $K_2^{x'} = K_1^{x'} = J_1$. Garel and Maillard (1983).
- (h) $\mu = 1$, $\nu = 2$, $K^x = |K^y|$, $K_2^y = -K_1^y$. The Odd model. Villain (1977a), André et al. (1979), Bryskin et al. (1980), Forgacs (1980).
- (i) $\mu = 2$, $\nu = 2$, $|K_1^y| = |K_1^x| = J$, $K_1^x = -J$, $K_1^{x'} = J$, $K_2^x = K_2^{x'} = J$, $K_1^y = -J$, $K_1^{y'} = J$, $K_2^y = K_2^{y'} = J$. The chessboard lattice, Bryskin et al. (1980).
- (j) f and i above could also be considered under periodic models with a diagonal symmetry direction, as in André et al. (1979).

Ground State Entropy

One consequence of frustration is the increase in the ground state degeneracy of the system. To illustrate: in Fig. 1, had all the bonds been equal to $+J$, the system would have had a unique ground state (all spins aligned), with the sole degeneracy associated with the overall (\pm) symmetry of the Hamiltonian. However, the frustrated system has an additional degeneracy associated with the breaking of a particular bond, e.g., a bond on any edge of the triangle may be broken, to yield the same ground state energy, $-J$. On a full lattice the effect is even more strikingly illustrated (Fig. 4).

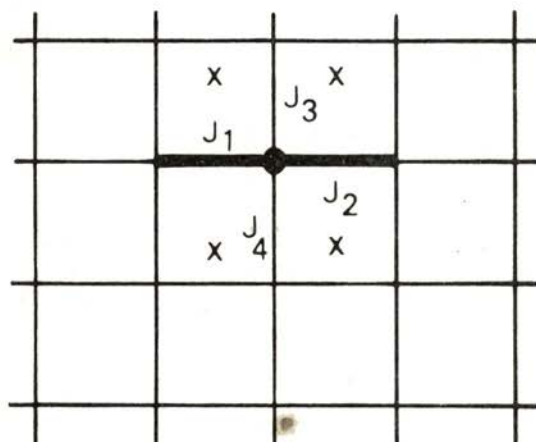


Fig. 4—The light bonds are FM, dark bonds AFM. The plaquettes marked with an 'x' are frustrated. The central spin indicated by a dark dot is effectively decoupled from the rest of the system, contributing a degeneracy of 2 to the ground state. In other words, the ground state is degenerate with respect to the breaking of the bonds J_1 and J_2 or J_3 and J_4 .

In an array, random or ordered, of frustrated plaquettes, there may be macroscopically many such spins, giving rise to a finite ground state entropy *per spin* (Binder 1980). Moreover,

there may be not only such single spins, but many-spin clusters under whose reversal the ground state entropy is invariant, giving rise to the cluster picture of spin glasses (Binder 1980, Miyashita and Suzuki 1981, Smith 1975, Soukoulis and Levin 1977), where one considers a system of uncoupled or loosely interacting clusters of spins who interact strongly within themselves. There is an interplay between dimensionality and ground state entropy that is remarkable; viz., not even all fully frustrated systems have finite ground state entropy (GSE) per spin. Both the triangular Ising AFM (Wannier 1950, Alexander and Pincus 1980) and the odd model of Villain (Villain 1977) have finite GSE, and no transition at finite temperatures. However their three dimensional counterparts, namely the Ising AFM on the fcc lattice and the FFSI in 3-d, have, respectively, ground state degeneracies of the order of $2^{N^{1/3}}$ (Danielian 1961) and $2^{N^{2/3}}$ (Chui et al. 1982) and thus zero GSE per spin. These models are thought to have, respectively, first order (Phani et al., 1979) and second order (Chui et al. 1982) transitions to an ordered low temperature phase ⁽¹⁾.

Although it is tempting to already try and draw conclusions with respect to the low temperature behaviour (existence or nonexistence of a phase transition, nature of the low temperature phase, etc.) from the existence or nonexistence of a finite rest entropy, it has been demonstrated (Hoever et al. 1981a) that this relationship is rather subtle. In particular, the existence of a finite rest entropy may or may not be accompanied by the absence or presence of a phase transition to an ordered phase at a finite temperature (see also Wolff, Hoever and Zittartz 1981).

Hoever et al. (1981a) have made the following conjecture: 'If all of the ground states (in the ensemble of ground states for the system) can be obtained one from the other by a succession of purely local transformations on the spins ($s \rightarrow -s$), then the global symmetry of the Hamiltonian (all $s \rightarrow -s$, uniformly) cannot be broken, i.e., there cannot be a phase transition to a phase with broken symmetry'. However, as they already point out,

⁽¹⁾ It has been claimed by Villain et al. (1980) that the AFM fcc Ising Model has a re-entrant paramagnetic phase at $T=0$. The results of Phani et al. (1979) are from Monte Carlo simulations. See also Binder (1980b).

the converse is not true, i.e., in the case where one needs to make some 'global' transformation to go from one ground state to another (in the sense that you have to flip over certain sets of 'rigid spins' (André et al. 1979) simultaneously) no decisive statement can be made. What makes the field so challenging is that most systems of interest happen to fall into this category! (see Fig. 5

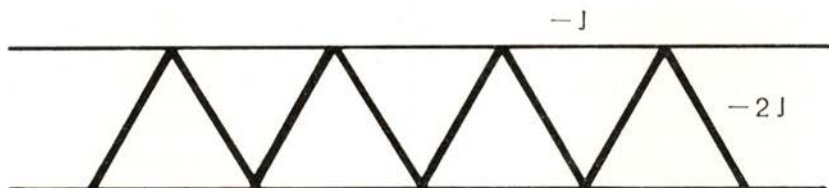


Fig. 5—As may be easily checked, even the extremely simple system of a triangular strip as shown in the figure, with Ising spins and AFM bonds, has sets of ground states which may be obtained one from the other by purely local transformations, as well as those that differ by 'global' transformations. This system has no phase transition even at zero temperature (de Nunes 1983).

and caption). Monte Carlo simulations of Ising systems on square or simple cubic lattices with a random distribution of \pm bonds have revealed precisely this kind of picture, with large (typically proportional to N) energy barriers between degenerate ground states or low-lying states (Malaspinas, Kirkpatrick 1977).

André et al. (1979) moreover hypothesize that if a phase transition exists in a frustrated system, it would be due to the internal field of the 'rigid spins' aligning the rest of the spins; thus, in a periodic frustrated system the ordered phase would necessarily reflect the periodicity of the 'rigid spins'. This implies that if there exists a transition to an ordered phase in a periodic frustrated system, it cannot be to a spin glass phase. Although the last part of this statement is supported by studies on layered frustrated models (see next paragraphs) the argument is not convincing. A similar assumption is employed by Chui et al. (1982) in constructing a Landau type argument for determining the nature of the phase transition encountered in the FFSI model in 3-d. However, if exact renormalization group (RG) transformations

on fully frustrated hierarchical lattices are any guide at all, we know that the ordering in the low temperature phase may be incommensurate with the underlying lattice, as evidenced by the chaotic RG trajectories. (Mc Kay et al. 1982, Svrakić et al. 1982, Derrida et al. 1983, Erzan 1983).

Derrida et al. (1978) have conjectured that for those frustrated models that have a transition temperature $T_c \neq 0$, there is a *negative* entropy associated with the formation of defects (negative interface entropy). The vanishing of the defect energy at $T = 0$ does not signal the absence of a phase transition, but the vanishing of the negative interface entropy does. They have checked their conjecture in the case of the anisotropic odd model (where the AFM couplings $-J'$ are taken so that $J' > J$, the FM couplings) and the anisotropic triangular AFM, where the AFM couplings in one direction are taken to be stronger than in the other two. In the latter case, $T_c = 0$ although the GSE per spin is zero, and the interface energy in the direction perpendicular to the anisotropy direction is finite; but the interface entropy is zero. In the anisotropic odd model they recover the results that $T_c \rightarrow 0$ as $J' \rightarrow J$; and they also show that the interface energy tends to zero in this limit as well.

An Exact Criticality Condition

Hoever et al. (1981) have treated random layered frustrated Ising models with translational invariance of both the horizontal and the vertical bonds in one direction, using transfer matrix methods. They have found that if the layering has a period of length ν , with n_+ and n_- being the total number of ferro- and antiferromagnetic couplings in the vertical direction within each period (the horizontal bonds were chosen to be ferromagnetic) ⁽¹⁾, the transition temperature depends only on the absolute value of the mean coupling, or, $|n_+ - n_-|/\nu$ and is otherwise independent of the particular distribution of bonds

⁽¹⁾ We will show in Section III that the free energy depends only on the distribution of the plaquette frustration functions ϕ_p (Eq. 2.3). Thus there is no loss of generality in this coiche; ϕ_p is invariant under all $K^x \rightarrow -K^x$.

within each period. Their results have been extended by Kardar and Berker (1982) and Wolff et al. (1981) to anisotropic random layered systems involving a distribution of magnitudes as well as signs of the coupling constants. The exact criticality condition is given by

$$\sum_{i=1}^{\nu} \tilde{K}_i^x = \left| \sum_{i=1}^{\nu} K_i^y \right|$$

where \tilde{K}_i^x is the dual (see section IV) of K_i^x and i is the row index. When the average vertical coupling within a strip is equal to zero, the transition temperature is depressed to zero.

For all other values of the average vertical coupling the transition is either to an antiferromagnetic or ferromagnetic phase depending upon the ratio of the horizontal and vertical couplings. The important thing to note is that the transition is of the ordinary Ising type, the specific heat has a logarithmic singularity, except in the case where ν is allowed to go to infinity, in which case one obtains an infinitely weak singularity (Hoever and Zittartz 1981, Mc Coy 1977). For the model with $K_i^x = K$; $K_i^y = K$, $i = 1 \dots m$, and $K_i^y = -K$, $i = m + 1, \dots, \nu$, $\nu = n + m$, Hoever and Zittartz (1981) find that if $n = m$, $T_c = 0$, the specific heat has a rounded maximum with respect to the temperature at some $T \neq 0$; and as $m \rightarrow \infty$ this maximum goes over to the logarithmic singularity of the Ising model. Their conjecture, that the rounded maximum signals 'local' ordering within the unfrustrated strips, effectively decoupled from each other by the frustrated layers, in the same spirit as the 'cluster' picture mentioned above, is remarkably born out by the behaviour of the specific heat reported from finite size scaling calculations made on strips of width m (Droz and Malaspinas 1982, Nightingale and Blöte 1980). On the other hand, for $n \neq m$, but $n/m \sim 1$, the amplitude of the logarithmic singularity is extremely small, and only a rounded maximum above T_c is really visible — caution to experimentalists! — quite indistinguishable from the smooth specific heat curves obtaining for $m = n$, or in the limit $\nu \rightarrow \infty$ (see also Longa and Olés 1980).

Besides coupling constant anisotropy, the introduction of an external field has been a fruitful approach to studying the effects

of 'fine tuning' (Toulouse 1980) frustration (Villain 1978, Penson et al. 1979). A third venue is provided by RG studies of hierarchical models (McKay et al. 1982, Svrakić et al. 1982, Erzan 1983) where the lattice structure, e.g. the coordination number, can be varied at will. However, there does not yet seem to be a universally applicable, quantitative measure of *competition*, comparable in elegance to the frustration function itself.

Ground State Energy

A way of tackling the problem of determining the ground state energy per spin in frustrated systems has been to define an average internal field (Derrida et al. 1979) equal to the difference between the number of satisfied and broken bonds incident on a spin, the average being taken over the ensemble of ground states. An amazing universality is displayed by this quantity, which is proportional to z , the coordination number of the lattice, for $d < 4$, and $z^{1/2}$ for $d \geq 4$ (Derrida et al. 1979, Alexander and Pincus 1980) for the fully frustrated lattices given in Fig. 2. Another universal feature of these lattices is the existence of a borderline dimensionality above which it is not possible to construct ground states such that only one bond is broken per each plaquette, i.e., the 'overblocking effect'. For the generalized fcc and FFSI lattices this borderline dimensionality is found to be four (Derrida et al. 1979).

The connection between ground state properties and the singularities of the free energy at $T > 0$ remains a subtle matter. Wolff et al. (1981) have shown for a random layered model, containing the odd model as a special case, that the critical surface as a function of the coupling constant anisotropy fails to reflect the discontinuities in the rest entropy, or the singularities (discontinuities in the slope) of the ground state energy surface. More recently, Garel and Maillard (1983) have demonstrated a remarkable fact: the partition function of a four parameter fully frustrated model ⁽¹⁾ (see Fig. 3g) is equivalent to the partition function of an anisotropic ferromagnetic model. The $T = 0$ point of

⁽¹⁾ This does not violate gauge invariance. The reduction in the number of parameters is what allows the mapping to be possible.

This is the case for the anisotropic triangular AFM (Stephenson 1970b) and those layered models where $\sum_i K_i^x \neq 0$ (Wolff and Zittartz 1982). The anisotropic triangular AFM has the further peculiarity that for some T_D , $T_c < T < T_D$, short range order of the above type obtains; however for $T > T_D$ the exponential decay of the correlation functions is modulated in the direction of the anisotropy axes by an oscillatory factor, with a temperature dependent wavelength (Stephenson 1970b).

Another class of fully frustrated systems is afforded by the checkerboard lattice (Bryskin et al. 1980, André et al. 1979) and the ff hexagonal and Kagomé lattices (Sütö 1981). For these 'superfrustrated' lattices (Sütö 1981) there is no quasi-LRO even at $T = 0$: the correlation length stays finite even at this temperature. Unfortunately, so far one cannot give a rule by which one may *a priori* decide if a lattice is superfrustrated or not. Bryskin et al. (1980) have given explicit expressions for the free energy, from which the zeroes of the partition function in the complex temperature plane may be calculated, for a partially frustrated lattice with a nonzero transition temperature, the odd model, and the checkerboard lattice. Work is in progress at this point for a full characterization of these systems via the distribution of the zeroes of their partition functions.

The effect of frustrations on the correlation functions of systems with a quenched random distribution of frustrations has been studied by various authors. Fradkin et al. (1978) have made a high temperature study of pair correlations and shown that the correlation functions decrease in the presence of frustrations ⁽¹⁾. Miyashita (1983) has considered the behaviour of correlations on frustrated lattices in 2-d, in the whole temperature range, depending on the relative positions of frustrated plaquettes with respect to the correlated spins. The results are extremely intriguing in that they reveal a non-monotonic suppression of correlations for certain configurations. This non-monotonicity of near-neighbour spin correlations had shown up in Migdal-Kadanoff type RG calculations on ff hierarchical lattices (Derrida et al. 1983, Erzan 1983) and was the origin of the novel RG behaviour (stable and unstable periodic RG trajectories) found in those models.

⁽¹⁾ See Section IV for further details.

Dilute Frustrated Systems

Another approach to the spin glass problem has been to investigate the effect of dilution on fully frustrated systems, or, alternatively, the effect of low concentrations of frustration on the properties of unfrustrated systems.

De Seze (1977) has given a phenomenological argument for the existence of a spin glass phase with a concentration dependent critical temperature in bipartite fully frustrated lattices ($T_c > 0$ for $x < 1$). Ono (1980) finds an ordered phase in a bond diluted AFM triangular 'cactus tree' in an intermediate concentration range. André et al. (1979) give an argument that for the diluted odd model the critical temperature remains at $T = 0$, and that the correlations will have the same power law decay as in the pure lattice.

Grest and Gabl (1979) have performed Monte Carlo computations on the triangular and fcc AFM lattices, and have found spin glass-like 'freezing' behaviour for concentrations above the percolation threshold. In the fcc lattice the transition to the AFM phase is first changed from first to second order, and then for $.8 < x < .4$ a phase appears with no LRO but strong hysteresis effects (The Edwards-Anderson order parameter has been calculated and shows slow decay). The prevailing wisdom in spin glass literature rules out a stable SG phase in 2-d, but not in 3-d (see, for example, Sherrington 1983).

De Nunes (1983) has performed a real space RG calculation on an AFM ff hierarchical lattice with bond dilution. At lower effective dimensionalities (or coordination number, z), the $T = 0$ critical point is destroyed by dilution, whereas for higher z one has a transition to an antiferromagnetically ordered phase. For these higher effective dimensionalities, at fixed concentration x , the recursion relations exhibit stable periods (rather than fixed points) in the low temperature region. The transition line terminates at some x bigger than the percolation threshold, at a critical point of infinite order.

The introduction of AFM bonds into an FM square lattice has been found (Vannimenus and Toulouse 1977) to destroy the FM transition at a concentration c of AFM bonds equal to .09. De Almeida et al. (1981) report a value of $c = .166$

obtained via an effective field approach. It is believed that the frustrated plaquettes percolate at this concentration (or an infinite string of frustrated plaquettes first appears). Miyashita and Suzuki (1981) have found a cluster (of rigid spins effectively decoupled from the rest by frustrated bonds) boundary percolation threshold at $c = .15$. For a triangular lattice the frustrated plaquette percolation threshold $c_f^* = .10 - .15$ (Sadiq et al. 1981). It is interesting to note that the concentration of frustrated plaquettes, c_f , shows a saturation effect, and stays nearly constant at about $1/2$, while c is varied above c_f^* , up to the percolation threshold for the FM bonds ($1/2$ for the square lattice; the situation is of course symmetric around this concentration). The ground state energy per spin is therefore rather insensitive to the variation of c above c_f^* (Kirkpatrick 1977).

Schuster (1979), by implementing methods to be outlined in section III, has shown that there is a further transition in the frustration network as a function of c . Namely, an infinite ladder of AFM bonds first appears at $c = .29$, leading to the possibility of isolated frustrations. His results have been corroborated by Kolan and Palmer (1980) using Monte Carlo methods. It still remains to be ascertained whether this transition in the frustration network is accompanied by a corresponding 'transition' in the behaviour of the spin system at $T > 0$. For a topological phase transition in a frustrated $x - y$ model, see Dzyaloshinskii and Obukov (1982).

III — GAUGE VARIABLES, GAUGE INVARIANCE AND THE FRUSTRATION FUNCTION

In the preceding section we have tried to give an overview of the phenomenology of frustrated systems. The methods employed to derive the results reported up to here were generalizations of methods applicable to conventional (unfrustrated) spin systems; in particular, transfer matrix methods, high temperature expansions (this last, however, making use of the gauge invariance and duality transformation concepts to be presented henceforth (Fradkin et al. 1978)), renormalization group analysis, and of course, Monte Carlo simulations. In this section we will introduce *gauge variables* as an extension of systems with spin degrees of freedom (Kadanoff 1976, Fradkin et al. 1978) and

the natural language in which to discuss 'bond randomness'. This allows us to extract the thermodynamically relevant features of an ensemble of frustrated systems, as well as allowing us to treat annealed and quenched bond randomness as part of one continuous picture.

Gauge Variables and Symmetries

We shall define *gauge variables* to be those variables that depend on two nearest neighbour site (vertex) indices on the lattice. As opposed to the *spin* variables which are located at the vertices of the lattice and depend on only one site index, the gauge variables can be thought of as variables living on the edges connecting the nearest neighbor sites. They are, then, a type of random variable custom made for representing a system of random interactions between nearest neighbor sites on a lattice. (Actually, the generalization to long range interactions as, for example, in the case of the infinite range spin glass, has also been made, Nishimori and Stephen 1983) Clearly, we can label the gauge variables ψ , either ψ_{ij} where i and j are site indices, or $\psi_{i,\mu}$ where i indicates a site and μ a particular lattice direction.

Let us recall that the Hamiltonian in (2.1)

$$H = - \sum_{(ij)} J_{ij} f(s_i, s_j)$$

is usually invariant under a set of symmetry operations

$$\{s_i\} \rightarrow \{s'_i\}. \quad (3.1)$$

The simplest example is the Ising model, where $s_i = \pm 1$, $f(s_i, s_j) = s_i s_j$, and the only nontrivial such symmetry operation consists of

$$\{s_i\} \rightarrow \{-s_i\}. \quad (3.2)$$

This is a *global* symmetry: the operation is applied to all the spins s_i in the system at once. We can easily construct other examples. The q -state Potts model has

$$f(s_i, s_j) = \delta_{s_i s_j} \quad (3.3)$$

where $\delta_{s_i s_j}$ is the Kroenecker delta and spins s_i can take on q different values. The relevant set of symmetry operations is obviously the group of permutations of q objects. We could, in fact, write the Potts spins (including the Ising model as the special case with $q = 2$) as q -dimensional vectors,

$$\mathbf{s}^\dagger(\mathbf{r}) = (s_1(\mathbf{r}), s_2(\mathbf{r}) \dots s_q(\mathbf{r})) \quad (3.4)$$

with $s_k(\mathbf{r}) = 0, 1$ and $\sum_k s_k(\mathbf{r}) = 1$. We can then express the permutation transformations as

$$s'_k(\mathbf{r}) = \sum_l M_{kl}^\alpha s_l(\mathbf{r}) \quad (3.5)$$

where the matrix M is a realization of the group of permutations of q objects, and α labels a particular element of this group. Following Kadanoff (1976), one can generalize this formulation to any set of spins $s(\mathbf{r})$ with some number (not necessarily discrete) of internal states, and the group of transformations between these states. Let us choose M to be a unitary representation. Then the simplest scalar that can be formed from these spins $\mathbf{s}(\mathbf{r})$, under the group of transformations M , is, in matrix notation,

$$f(\mathbf{s}(\mathbf{r}), \mathbf{s}(\mathbf{r}')) = \mathbf{s}^\dagger(\mathbf{r}) (M^\alpha)^{-1} M^\alpha \mathbf{s}(\mathbf{r}') \quad (3.6)$$

where \mathbf{r}, \mathbf{r}' label lattice sites. Note that the particular element of the group, α , employed, is taken to be independent of \mathbf{r} , and the resulting Hamiltonian is invariant under this *global* transformation (3.5).

Now let us consider a more general form of interactions between generalized spins residing at the lattice sites \mathbf{r}, \mathbf{r}' , which may depend not only on the lattice sites \mathbf{r}, \mathbf{r}' , but also on the internal states of the spins at those sites, and must have the matrix form $\psi_{kl}(\mathbf{r}, \mathbf{r}')$ where k, l label the internal states of the spins at \mathbf{r}, \mathbf{r}' . In matrix notation,

$$H = -J \sum_{(\mathbf{r}, \mathbf{r}')} \mathbf{s}^\dagger(\mathbf{r}) \psi(\mathbf{r}, \mathbf{r}') \mathbf{s}(\mathbf{r}') \quad (3.7)$$

The simplest example is again the Ising model, where

$$\mathbf{s}(\mathbf{r}) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ or } \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{3.8}$$

and

$$\psi(\mathbf{r}, \mathbf{r}') = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ or } \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

the first giving rise to FM, the second to AFM interactions. If the spins in (3.7) are Potts spins as defined in eq. (3.4), and the $\psi(\mathbf{r}, \mathbf{r}')$ then elements of the group of permutations of q objects (traceless except for the identity element), the Hamiltonian (3.7) represents a random vector Potts model ⁽¹⁾. (Nishimori and Stephen 1983. These authors use a one dimensional representation of the symmetry group).

These (matrix) variables $\psi(\mathbf{r}, \mathbf{r}')$ which can be thought of as residing on the bonds connecting the lattice sites \mathbf{r}, \mathbf{r}' , we shall call gauge variables. They, in turn, transform under *gauge transformations*, which one can write

$$\psi'_{mn}(\mathbf{r}, \mathbf{r}') = \sum_{kl} M_{mk}^{\alpha(\mathbf{r})} \psi_{kl}(\mathbf{r}, \mathbf{r}') (M_{ln}^{\alpha(\mathbf{r}')})^{-1} \tag{3.9}$$

Note that here one has the extra freedom of allowing the particular element α of the symmetry group to depend on \mathbf{r}, \mathbf{r}' . One may

⁽¹⁾ In Nishimori and Stephen's (1983) notation, the Hamiltonian is given by

$$H = -J \sum_{(ij)} \delta(\sigma_i - \sigma_j + r_{ij}) = - \sum_{(ij)} \sum_p J_{ij}^p \exp(2\pi i(\sigma_i - \sigma_j)p/q)$$

where $J_{ij} = \exp(2\pi i r_{ij}/q)$, $r_{ij} = 0, 1, \dots, q-1$ may have any desired distribution. Clearly, $r_{ij} = 0$ reduces to the FM Potts model. $r_{ij} \neq 0$ constrains spins on adjacent sites i, j to be in states differing by r_{ij} . The AFM Potts model is equivalent to taking

$$H = \sum_{(ij)} \sum_{r \neq 0} \sum_p J_{ij}^p \exp(2\pi i(\sigma_i - \sigma_j)p/q)$$

(This model also correctly reduces to the Ising model for $q=2$). The cyclic matrices ψ in the matrix representation above are given explicitly by $\psi_{kl}(ij) = \delta_{k, l+r_{ij}}$, $l+r_{ij} = l+r_{ij}-q$; $r_{ij} = 0, \dots, q-1$; $k, l = 1, \dots, q$.

construct scalars from these gauge variables, that will be invariant under the (*local*) gauge transformation (3.9). The simplest such scalar is the *trace* of products of $\psi(\mathbf{r}, \mathbf{r}')$, such that $\mathbf{r}_1, \mathbf{r}_2, \dots$ form a closed loop, and where we have again taken M to be unitary (Kadanoff 1976); see Fig. 6.

$$\begin{aligned} \hat{f}_\Gamma(\psi) &= \text{Tr } \psi(\mathbf{r}_1, \mathbf{r}_2) \psi(\mathbf{r}_2, \mathbf{r}_3) \dots \psi(\mathbf{r}_n, \mathbf{r}_1) \\ &= \text{Tr } M^{\alpha(\mathbf{r}_1)} \psi(\mathbf{r}_1, \mathbf{r}_2) (M^{\alpha(\mathbf{r}_2)})^{-1} M^{\alpha(\mathbf{r}_2)} \dots \psi(\mathbf{r}_n, \mathbf{r}_1) (M^{\alpha(\mathbf{r}_1)})^{-1} \end{aligned} \quad (3.10)$$

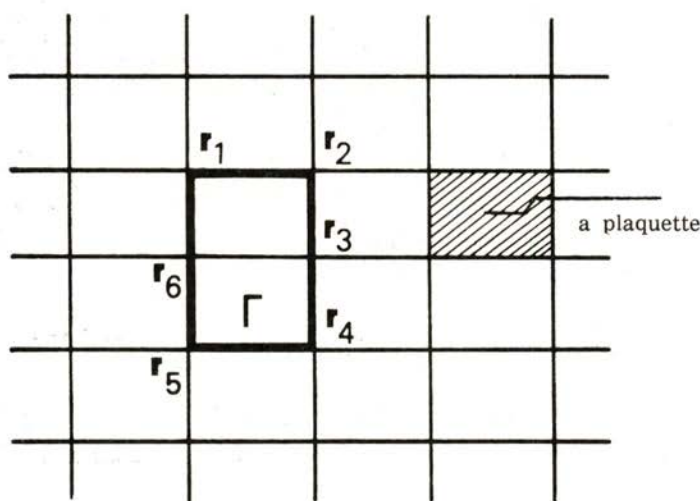


Fig. 6 — Γ labels the path formed by the bonds $(\mathbf{r}_1, \mathbf{r}_2), (\mathbf{r}_2, \mathbf{r}_3) \dots (\mathbf{r}_6, \mathbf{r}_1)$. See Eq. (3.10).

The smallest such loop Γ that may be formed on any given lattice is what is called a *plaquette*. Therefore, the simplest gauge-invariant objects we can construct out of the gauge variables, live on plaquettes (as opposed to the functions (3.6) formed from spin variables, which are invariant under global transformations, and live on bonds).

In the case of the Potts model ⁽¹⁾ (with $q > 1$) let us define

$$\phi_p \equiv (\text{Tr } \prod_p \psi - 1) / (q - 1) \quad (3.11)$$

where $\prod_p \psi$ denotes the (matrix) product of the ψ variables around the plaquette p . The function ϕ_p may be taken as the frustration function for the (vector) Potts model ⁽¹⁾ with

$$\phi_p = \begin{cases} -1 / (q - 1) & \text{plaquette frustrated} \\ 1 & \text{'' unfrustrated.} \end{cases}$$

Obviously, ϕ_p is invariant under the transformation (3.9). For $q = 2$, ϕ_p reduces to the plaquette frustration function as defined by Toulouse (1977) using a one dimensional representation of the symmetry group Z_2 of the Ising model ⁽²⁾.

Symmetries of the Partition Function

After Kadanoff (1976) we shall call those representations of the symmetry groups of the spin and gauge variables *simple*, where one may write

$$\text{Tr}_s f(\mathbf{s}) = \sum_{\alpha} f(M^{\alpha} \mathbf{s}) \tag{3.12}$$

and

$$\text{Tr}_{\psi} \hat{f}(\psi) = \sum_{\alpha} \hat{f}(M^{\alpha} \psi)$$

where f, \hat{f} are some function of the variables. Thus, if we have chosen simple representations for our spin and gauge variables,

⁽¹⁾ Clearly this choice is not unique.

⁽²⁾ In taking such a one dimensional representation of the symmetry group Z_N , the form of Eq. (3.9) should be kept in mind, since it implies a constraint on the transformations that may be performed on a string of gauge variables forming a loop. E.g., in Fig. 1a, b, 'flipping' all the bonds simultaneously (multiplying each bond by -1) is not an allowed gauge transformation, as will be immediately seen if one takes care to write

$$J'_{ij} = M(i) J_{ij} M(j)^{-1}$$

where $i, j = 1, 2, 3$ are the vertices of the triangle, $M(i) = \pm 1$, $M(i)^{-1} = M(i)$. However, Fig. 1 a and b are related by a gauge transformation, where $M(1) = M(2) = -1$, $M(3) = 1$. Notice that the frustration function for this loop is again invariant under this transformation.

we may write the partition function of a quenched random bond system as

$$Z = \sum_{\{\alpha(\mathbf{r})\}} \exp \left[K \sum_{(\mathbf{r}, \mathbf{r}')} \mathbf{s}(\mathbf{r})^\dagger (M^{\alpha(\mathbf{r})})^{-1} \psi(\mathbf{r}, \mathbf{r}') M^{\alpha(\mathbf{r}')} \mathbf{s}(\mathbf{r}') \right] \quad (3.13)$$

where $K = \beta J$.

Now notice that Z is invariant under the set of gauge transformations (eq. 3.9)

$$\psi(\mathbf{r}, \mathbf{r}') \rightarrow M^{\alpha(\mathbf{r})} \psi(\mathbf{r}, \mathbf{r}') (M^{\alpha(\mathbf{r}')})^{-1}.$$

Thus we have our first result that the partition functions of two spin systems on lattices whose bond configurations may be obtained one from the other by a set of transformations (3.9) for some $\{\alpha(\mathbf{r})\}$, are equal (Fradkin et al. 1978).

A further symmetry of the partition function and, furthermore, of the (field free) *Hamiltonian*, is given by the following local transformation that affects not only the gauge variables impinging upon a particular site \mathbf{r} , but also the spin variable at that site

$$\begin{aligned} \psi(\mathbf{r}, \mathbf{r}') &\rightarrow M^{\alpha(\mathbf{r})} \psi(\mathbf{r}, \mathbf{r}') I \\ \mathbf{s}(\mathbf{r}) &\rightarrow \mathbf{s}(\mathbf{r}) [M^{\alpha(\mathbf{r})}]^{-1} \end{aligned} \quad (3.13a)$$

where I is the identity matrix. (In the more familiar language of the Ising model, this would, for example, correspond to reversing the sign of all the bonds impinging on \mathbf{r} , and redefining the spin at \mathbf{r} such that $s \rightarrow -s$). This *mixed* transformation is not needed for the development in this section, but in Section IV, when dealing with correlation functions, we will see that the correlation functions $\langle s(\mathbf{r}) s(\mathbf{r}') \rangle$ are not invariant under a mixed gauge transformation performed at the site \mathbf{r} or \mathbf{r}' , and therefore we have to consider slightly more generalized objects.

It follows immediately from this invariance, that the partition function of a quenched random bond system must depend only on those sets of quantities (constructed from gauge variables) that are scalars under such transformations, and the partition function may be labeled by this set of quantities. We have already constructed such a quantity in Eqs. (3.10, 3.11) and for q -state Potts models we have shown that it is the direct generalization

of the frustration function of Toulouse for the Ising case. Thus, for a quenched random system we may write

$$Z = Z \{ \phi_p \} \quad (3.14)$$

where p runs over all the plaquettes of the lattice. This is a rather remarkable fact. In particular, it leads, e.g. on the square lattice, to the simplification, that one may treat, instead of a system with a completely random distribution (magnitudes being held fixed), one where, say, the horizontal bonds are taken to be all of the same sign, and the vertical bonds are chosen randomly, since any distribution of ϕ_p may be realized in this way (Hoever et al. 1981a).

Another immediate consequence of Eq. (3.13) is that Z can be written

$$Z = \sum_{\{ \alpha(r) \}} \exp [K \sum_{(r, r')} \mathbf{s}_0^\dagger (M^{\alpha(r)})^{-1} \psi(r, r') M^{\alpha(r')} \mathbf{s}_0] \quad (3.15)$$

where \mathbf{s}_0 is an arbitrarily chosen state of the variables $\mathbf{s}(r)$, which leads to (via Eq. 3.12)

$$Z \{ \phi_p \} = \Omega_M \sum'_{\{ \psi \}} \exp [K \sum_{(r, r')} \mathbf{s}_0^\dagger \psi(r, r') \mathbf{s}_0] \quad (3.16)$$

where Ω_M is the 'volume' of the group of transformations M at each site (e.g. for the Z_2 symmetric Ising model, this is just 2^N), and where the prime on the sum indicates that the sum over the ψ is restricted to those configurations of ψ that give the same distribution of plaquette functions ϕ_p . Without this constraint, we clearly have the partition function of the *annealed* system. We may express this constraint by means of delta functions, viz.,

$$Z \{ \phi_p \} = \Omega_M \sum_{\{ \psi \}} \prod_p \delta [\phi_p - (\text{Tr} \prod_p \psi - 1) / (q - 1)] \cdot \exp [K \sum_{(r, r')} \psi_{00}(r, r')] \quad (3.17)$$

where $\psi_{00} = \mathbf{s}_0^\dagger \psi \mathbf{s}_0$. If we can construct some \tilde{f}_p such that

$$\tilde{f}_p > 0 \quad \phi_p = (\text{Tr} \prod_p \psi - 1) / (q - 1) \quad (3.18)$$

$$\tilde{f}_p < 0 \quad \phi_p \neq (\text{Tr} \prod_p \psi - 1) / (q - 1)$$

the ψ being the integration variables and ϕ_p now a fixed set of numbers for the plaquettes p , then we could write (Fradkin et al. 1978)

$$Z \{ \phi_p \} = \Omega_M \lim_{K_p \rightarrow \infty} \sum_{\{ \psi \}} \exp [K \sum_{r,r'} \psi_{00}(r, r') + K_p \sum_p \tilde{f}_p] \quad (3.19)$$

For the Potts model, with definition (3.11), we may take

$$\tilde{f}_p = \phi_p (\text{Tr} \prod_p \psi - 1) / (q - 1) \quad (3.20)$$

Notice that this has the interesting (and foreseeable) consequence that as $q \rightarrow \infty$, those configurations which are frustrated contribute to Z with a vanishing weight compared to those that are not, i.e., in this limit, with $K_p \rightarrow \infty$, the model becomes completely unfrustrated.

Some comments as to the consequences of Eq (3.19) are in order. For instance, Toulouse and Vannimenus (1980) have proposed a 'restricted annealing scheme' where, instead of inserting the delta-functions in Eq. (3.17), one takes

$$Z = \Omega_M \sum_{\{ \psi \}} \exp [K \sum_{r,r'} \psi_{00} + K_p \sum_p \phi_p] \quad (3.21)$$

with the constraint that

$$\partial \ln Z / \partial K_p = \langle \sum_p \phi_p \rangle = 0 \quad (3.22)$$

($K_p = 0$ is, of course, the annealed model). In the Ising case, which they treat, this corresponds to a constrained — annealed system with an equal number of frustrated and unfrustrated plaquettes. Since this is also expected to be true of the quenched model with an equal number of \pm bonds, on the average, this provides a first order approximation to the properties of the quenched system. With our definition of the frustration function for the Potts model, this same approximation holds true, for a distribution of couplings (in the one dimensional representation) given by

$$\begin{aligned} J_{ij} &= J && \text{with probability } p \\ J_{ij} &= J \exp(2\pi i r / q) && \text{'' '' } (1-p) / (q-1) \\ &&& (r = 1, 2, \dots, q-1) \end{aligned} \quad (3.23)$$

The solution of Eq. (3.22) in the space of K, K_p (a solution exists only for $K_p < 0$) defines a subset, then, of models with spin and gauge coupling terms, which approximate the quenched random frustrated spin models in some sense. Note that the limit $K_p \rightarrow \infty$ gives the pure Potts partition function. The limit $K_p \rightarrow -\infty$ gives the *fully* frustrated system. The line (3.22) interpolates between the annealed and the fully frustrated cases (Toulouse and Vannimenus 1980, Toulouse 1980). It would be interesting to work out how this line actually behaves for different models in d dimensions. Toulouse and Vannimenus (1980) ask the question whether it intersects any phase transition lines in the $K, -K_p$ space. This would be an approximation to a SG transition. One would also like to know if there is another transition on the $K_p \rightarrow -\infty$ line and whether the $\langle \sum_p \phi_p \rangle = 0$ line comes close to this in some way, as, say, the dimensionality is raised. Do the two transitions (if there are two) merge? This would be a step in the direction of the conjecture of Alexander and Pincus (1980) that the SG transition might become 'like' a transition in ff systems at high enough dimensionality.

Quenched Averages

Clearly, now, the task of taking 'quenched averages', or averaging the observables over all possible realizations of the (bond) randomness is simplified to a great extent, since one does not have to take into account each such possible realization but only those that differ from each other in a gauge invariant way, namely, those that give rise to distinct distributions of the generalized frustration function ϕ_p . These configurations will then have to be weighted by the probability of occurrence of $\{\phi_p\}$ namely by $P\{\phi_p\}$, given a certain distribution $P\{\psi\}$. Let us write this (Fradkin et al. 1978, Schuster 1979)

$$\langle Q \rangle = \sum_{\{\phi_p\}} P\{\phi_p\} Q\{\phi_p\} \quad (3.24)$$

where Q is any gauge independent quantity, and $\langle \rangle$ indicates a quenched average. Now one has to determine $P\{\phi_p\}$. Let us

assume that each bond (gauge) variable is distributed independently with a probability $p_{r, r'}(\psi)$. Then,

$$\begin{aligned} P\{\phi_p\} &= \frac{\sum'_{\{\psi\}} P\{\psi\}}{\sum_{\{\psi\}} P\{\psi\}} \\ &= \frac{\sum'_{\{\psi\}} \prod_{(r, r')} p_{r, r'}(\psi)}{\sum_{\{\psi\}} \prod_{(r, r')} p_{r, r'}(\psi)} \\ &= \frac{\sum'_{\{\psi\}} \exp\left[\sum_{(r, r')} \ln p_{r, r'}(\psi)\right]}{\sum_{\{\psi\}} \exp\left[\sum_{(r, r')} \ln p_{r, r'}(\psi)\right]} \end{aligned}$$

where the prime indicates that the sum includes only those configurations of ψ that give rise to $\{\phi_p\}$. Let us again consider

$$f_0 \equiv s_0 \psi(r, r') s_0$$

Notice that if we have a distribution for the ψ such that $p_{r, r'}(\psi)$ is independent of r, r' , and for example,

$$p(\psi) = \tilde{p}(f_0) = \begin{cases} x & f_0 = 1 \\ x-1 & f_0 = 0 \end{cases} \quad (3.25)$$

we may write,

$$\tilde{p}(f_0) = \rho^{1/2} \exp[K_f(f_0 - 1/2)] \quad (3.26)$$

where,

$$\rho = x(1-x), \quad K_f = \ln[x/(1-x)] \quad (3.27)$$

with the result that

$$P\{\phi_p\} = \frac{\sum'_{\{\psi\}} \exp[K_f \sum_{r, r'} f_0(r, r')]}{\sum_{\{\psi\}} \exp[K_f \sum_{r, r'} f_0(r, r')]} \quad (3.28)$$

Factors of $\rho \exp(-K_f)$ have cancelled from the numerator and denominator: One immediately sees that $P\{\phi_p\}$ is nothing but the ratio of the partition functions of the original spin system in the fixed gauge with all the $s(r) = s_0$ (see Eq. 3.16), i.e.,

$$P\{\phi_p\} = \frac{Z\{\phi_p\}_{K_f}}{Z\{\phi_p\}_{K_f}} \quad (3.29)$$

with the effective coupling constant (temperature) given by Eq. (3.27) (Fradkin et al. 1978, Schuster 1979).

Nishimori (1981) has noticed that this form of $P \{ \phi_p \}$ together with Eq. (3.24) allows one to rigorously calculate the internal energy, and obtain bounds on the specific heat and correlation functions, on a subspace of the phase diagram given by $K_f = K$. This leads to constraints on the form of the PM - SG - FM phase boundaries. (Nishimori 1981, Nishimori and Stephen 1983).

To calculate $P \{ \phi_p \}$ is not a trivial matter. In the next section, we will see that if $\{ \phi_p \}$ has n frustrations, this task is equivalent to calculating an n -point correlation function in the system dual to the original system. This is certainly no great simplification! However, there are certain results that are accessible, as we shall see.

IV — DUALITY TRANSFORMATIONS

Duality is essentially a geometrical concept. Since we are dealing with statistical mechanical models on lattices, it is useful to introduce the notion of a *simplex* as an s dimensional element of the lattice in d dimensions. Thus, a point (vertex) has simplex number 0, a bond (edge) has simplex number 1, a plaquette 2, and an elementary volume, simplex number 3, etc. The *dual* to any lattice can be constructed by 'intersecting' each element of simplex number s of the original lattice by a simplex of dimensionality $\tilde{s} = d - s$. (It is easy to convince oneself, that for a hypercubic lattice, where the dual can be obtained simply by displacing the lattice by $1/2$ the lattice spacing in the (111...) direction, the above scheme holds. Thus, e.g., in 3d, each vertex ($s = 0$) of the original lattice is surrounded by a cube ($\tilde{s} = 3$), each bond ($s = 1$) is intersected by a plaquette ($\tilde{s} = 2$) and each plaquette ($s = 2$) is in turn intersected by a bond of the dual lattice ($\tilde{s} = 1$) etc.) (Savit 1980).

Statistical mechanical models may be characterized by a simplex number s (Savit 1980, Toulouse 1980). The terms appearing in the Hamiltonian — invariants constructed from objects (spins, gauge variables etc.) living on simplices of dimension s — are

obtained by multiplying together such objects bounding a simplex of dimension $s + 1$, on the given lattice. Thus in Eq. (3.6), spin-spin interactions involve a product of spins at the two ends of a bond, and the invariant constructed from gauge variables (Eq. 3.10) involves a product of gauge variables around a plaquette of the given lattice.

Duality transformations are exact transformations that map a theory with simplex number s into one with simplex number $\bar{s} = d - s$, in such a way that the partition functions of the two theories are simply proportional to each other, with a temperature dependent proportionality factor, and the temperature (coupling constant) of the dual theory is a monotone decreasing function of the first (In those theories that are self-dual — e.g. the Ising and Potts models on square lattices — this provides a unique way of determining the critical temperature).

Duality transformations for the Ising model (Kadanoff and Ceva 1971, Wegner 1971), Ising model with gauge coupling term (Balian et al. 1975), models with Z_N and $U(1)$ symmetry (Savit 1980) and the ordinary Potts model (Wu 1982) have already been extensively treated in the literature. What I propose to do here is to illustrate the basic ideas by deriving the duality transformation for the 2d Ising model with a gauge coupling term (The generalization of this to vector Potts models is given in the Appendix). Then I will discuss the concept of *disorder variables* and show how the partition function of a model with n frustrations (Eq. 3.29) is related to an n -point (disorder-disorder) *correlation function* in the dual model. I will then consider *gauge invariant correlation functions* and a few remarks about their asymptotic behaviour and phase transitions will follow.

The Two-Dimensional Ising model

Following Balian et al. (1975) let us consider the partition function in Eq. (3.19) with a finite gauge coupling constant K_p . We may represent the gauge variables by $A_{ij} = \pm 1$ in this case, and write, with the choice all $s_i = 1$, up to numerical factors,

$$Z = \sum_{\{A_{ij}\}} \exp [K \sum_{(ij)} A_{ij} + K_p \sum_p \prod_p A_{ij}] \quad (4.1)$$

where $\prod_p A_{ij}$ indicates a product of the gauge variables around the plaquette p , and \sum_p runs over all plaquettes. Note that we have set all the frustration functions $\phi_p = 1$ for the time being, i.e., we are dealing with an unfrustrated system. Writing

$$\exp(KA_{ij}) = \cosh K (1 + A_{ij} \tanh K) \quad (4.2)$$

$$\exp(K_p \prod_p A_{ij}) = \cosh K_p (1 + \prod_p A_{ij} \tanh K_p)$$

Z becomes

$$Z = (\cosh K)^E (\cosh K_p)^N \sum_{\{A_{ij}\}^1} \prod_p (1 + A_{ij} \tanh K) \prod_p (1 + \prod_p A_{ij} \tanh K_p) \quad (4.3)$$

where N and E are the total number of sites and edges on the lattice, $\tilde{\prod}_p$ denotes a product over all plaquettes and \prod_l denotes a product over all links (i, j) . We may represent the result of expanding the products as a sum over graphs G on a lattice consisting of all distributions of plaquettes p and edges l on the lattice, \mathcal{L} ,

$$\prod_l (1 + A_{ij} \tanh K) \tilde{\prod}_p (1 + \prod_p A_{ij} \tanh K_p) = \sum_{G \subset \mathcal{L}} \prod_{l \subset G} A_{ij} \tanh K \tilde{\prod}_{p \subset \mathcal{L}} (\prod_p A_{ij}) \tanh K_p \quad (4.4)$$

Now it is easy to see that as a result of the trace in Eq. (4.3), only those terms will survive where each plaquette edge is shared between two plaquettes, or coincides with a link l , and is not shared by other plaquettes. This gives

$$Z = (\cosh K)^E (\cosh K_p)^N \sum_{G \subset \mathcal{L}} (\tanh K)^L (\tanh K_p)^P \quad (4.5)$$

where P is the total number of such plaquettes and L the total length of the boundary of the clusters of plaquettes, i.e., the total number of plaquette edges that belong to only one plaquette. Now we can construct \mathcal{L}_D , the dual graph to \mathcal{L} , and make a one to one correspondance with spin variables located on \mathcal{L}_D with the

graphical elements of G . Thus we shall stipulate that if a plaquette on \mathcal{L} belongs to G , then a spin residing at the site dual to this plaquette on \mathcal{L}_D , has the value $s_{\tilde{i}} = -1$, and if not, $s_{\tilde{i}} = +1$. Thus we have

$$P = \sum_{\tilde{i}} (1 - s_{\tilde{i}}) / 2 \quad (4.6)$$

where \tilde{i} now runs over the sites of \mathcal{L}_D . This gives us automatically

$$L = \sum_{(\tilde{i}, \tilde{j})} (1 - s_{\tilde{i}} s_{\tilde{j}}) / 2 \quad (4.7)$$

where the (\tilde{i}, \tilde{j}) are the adges of \mathcal{L}_D , and each of them intersects an edge of \mathcal{L} . Clearly, Eq. (4.7) holds, because the product $s_{\tilde{i}} s_{\tilde{j}}$ is positive for (\tilde{i}, \tilde{j}) crossing any link on \mathcal{L} that is shared by two plaquettes on G , and is only negative if this link happens to be on the boundary of a cluster of plaquettes on G . Finally we have

$$Z = (\cosh K)^E (\cosh K_p)^N \sum_{\{s_{\tilde{i}}\}} \left\{ \exp \left[\frac{1}{2} \ln \tanh K \sum_{(\tilde{i}, \tilde{j})} (1 - s_{\tilde{i}} s_{\tilde{j}}) \right] \right. \\ \left. \cdot \exp \left[\frac{1}{2} \ln \tanh K_p \sum_{\tilde{i}} (1 - s_{\tilde{i}}) \right] \right\}$$

which we may write

$$Z = (\cosh K)^E (\cosh K_p)^N \cdot \sum_{\{s_{\tilde{i}}\}} \exp \left[K^* \sum_{(\tilde{i}, \tilde{j})} (s_{\tilde{i}} s_{\tilde{j}} - 1) \right. \\ \left. + h \sum_{\tilde{i}} (s_{\tilde{i}} - 1) \right] \quad (4.8)$$

where

$$K^* = -1/2 \ln \tanh K \quad (4.9) \\ h = -1/2 \ln \tanh K_p$$

are the dual couplings (inverse temperatures). Observe that the term in Eq. (4.1), of simplex number 1 has given rise to another such term, and the gauge coupling ($s = 2$) has given rise to a field term, with $\tilde{s} = d - 2 = 0$. The transformation in 3d proceeds in like manner (Balian et al. 1975) where now the terms of the form $\sum_{ij} A_{ij}$ generate plaquette couplings and vice versa.

endpoints. It is easy to convince oneself that it is possible to deform this path arbitrarily, by performing a series of gauge transformations on the dual lattice. However, the correlation functions, unlike the partition function, are *not* invariant under the full mixed transformation, Eq. (3.13a), performed on the gauge variables impinging on \tilde{i} or $\tilde{i} + r$ and the spins at these points.

In the more familiar language of the Ising model, the transformation

$$s_{\tilde{i}} \rightarrow (-1) s_{\tilde{i}}$$

$$A_{\tilde{i}, \tilde{i} + \mu} \rightarrow (-1) A_{\tilde{i}, \tilde{i} + \mu}$$

gives out a factor of (-1) in front of Eq. (4.18) (Fradkin et al. 1978, Savit 1980).

Gauge Invariant Correlation Functions

Having obtained a recipe (Eq. 3.24) for calculating quenched averages of gauge invariant quantities, let us proceed to construct the gauge invariant correlation functions for the Ising model in two and three dimensions. In two dimensions one has,

$$\langle s_i \prod_{\Gamma_{ij}} A_{kl} s_j \rangle \xrightarrow[\text{in a system with } n \text{ frustrations}]{\text{Duality}} \text{n-point correlation function in a system with two frustrations at the plaquettes dual to } i, j. \quad (4.23)$$

where Γ_{ij} is now a *closed loop* going through the points i, j (Fradkin et al. 1978, Savit 1980). In three dimensions, the correlation function

$$\langle \prod_p A \prod_{p'} A \rangle$$

where p, p' are two different plaquettes is a gauge invariant quantity. But it turns out that the following object leads to more interesting results. For a pure gauge coupling theory, take any *loop* Γ and take the product of the plaquette functions lying on

any surface bounded by this loop. In the Ising case, with $A_{ij}^2 = 1$ clearly only the gauge variables lying on the loop Γ itself survive. The correlation function

$$\langle \prod_{\Gamma} A \rangle \xrightarrow{\text{Duality}} \frac{\text{Partition function of the 3d Ising spin system with all the bonds intersecting the surface bounded by } \Gamma, \text{ reversed.}}{\text{Partition function of the unfrustrated system.}} \quad (4.24)$$

Fradkin et al. 1978, Savit 1980). Note that the configuration of bonds described in the numerator of the RHS of (4.24) corresponds, for a system originally without frustrations, to the creation of a closed loop of frustrations threaded by Γ . The form of Eq. (4.24) again allows one to calculate the excess free energy due to such a closed tube of frustrations, the simplest configuration of frustrations possible in 3d. In the high and low temperature limits, respectively, of the dual (gauge) model, one has

$$\Delta F \sim \begin{cases} \alpha_1 A_{\Gamma} / K & K > K_c \\ \alpha_2 L_{\Gamma} / K & K < K_c \end{cases} \quad (4.25)$$

where α_1, α_2 are temperature dependent coefficients, A_{Γ} and L_{Γ} are the minimal area enclosed by Γ and the perimeter of Γ . K_c is the critical coupling of the 3-d Ising model (Fradkin et al. 1978).

Phase Transitions in the Frustration System

Let us go back to the probability of finding a certain configuration of frustrations in an ensemble of random configurations of bonds. Consider the normalized probability (Schuster 1979)

$$P \{ \phi_p \} / P \{ \phi \equiv 1 \} = Z \{ \phi_p \}_{K_f} / Z \{ \phi \equiv 1 \}_{K_f} \quad (4.26)$$

by Eq. (3.29). Clearly, the RHS is the same as Eq. (4.13), for a 2d Ising system, with K_f being the dual temperature to K^* .

path $\Gamma_{\tilde{i}, \tilde{i}+r}$ on the dual lattice gives rise to two frustrations precisely at those plaquettes dual to \tilde{i} and $\tilde{i}+r$. This construction can be generalized to any $2n$ -point correlation function. Paths connecting these points pairwise will give rise, in the dual lattice, to n pairs of frustrations (Fradkin et al., Savit 1980). Thus we are back to the picture in the previous subsection, Eq. (4.13) and the following paragraph. Note, however, the added twist: the disorder-disorder correlation function of the Ising model in 2d is found to be equal to the partition of the model with frustrations located at the plaquettes dual to the disorder variables, normalized by the partition function of the unfrustrated model. One could equally well say that the disorder variables act as *sources* and *sinks* of *defects* within an ordered system (see Fig. 7). On the

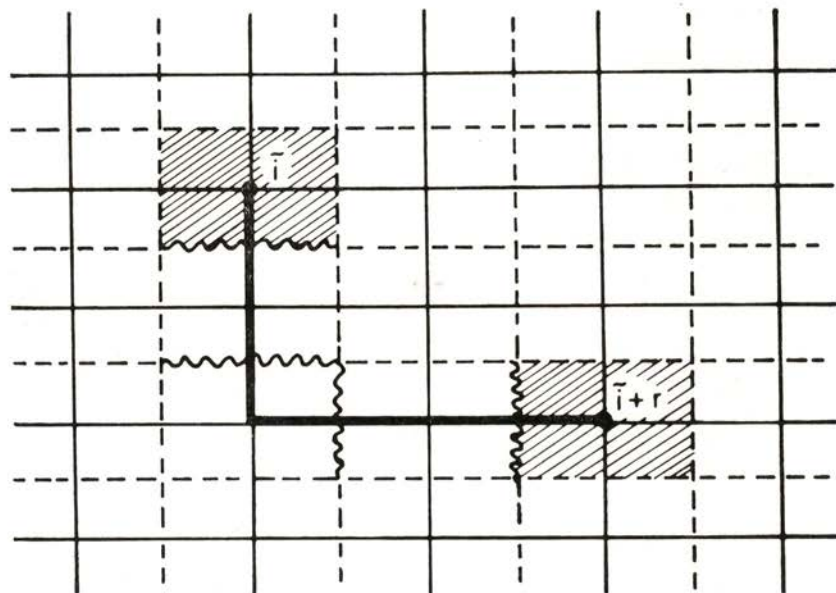


Fig. 7—A path (heavy line) $\Gamma_{\tilde{i}, \tilde{i}+r}$ connects the disorder variables $\sigma_{\tilde{i}}, \sigma_{\tilde{i}+r}$ on the original lattice. The dual lattice (dashed lines) has the signs of the links dual to Γ reversed (wiggly lines). The shaded plaquettes on the dual lattice are frustrated.

dual system, the dual path of reversed couplings costs ground state energy proportional to the length of the path Γ (see Fradkin et al. for a detailed discussion).

In the 2d Potts model, a similar (though not quite identical) picture emerges. The relevant two point correlation function is

$$(q-1)^{-1} \cdot \langle q \delta_{\sigma_{\tilde{i}} \sigma_{\tilde{i}+r}} - 1 \rangle = Z^{-1} \sum_{\tilde{G} \subset \mathcal{L}} u^{b(\tilde{G})} q^{n(\tilde{G})} \quad (4.20)$$

where $u = e^K - 1$, \tilde{G} are all possible graphs in \mathcal{L} , consisting of points and edges such that they contain a continuous path connecting the points \tilde{i} , $\tilde{i} + r$, $b(\tilde{G})$ and $n(\tilde{G})$ are the number of edges and connected parts of \tilde{G} , respectively. Performing the duality transformation on the RHS of (4.20), one obtains

$$(q-1)^{-1} \cdot \langle q \delta_{\sigma_{\tilde{i}} \sigma_{\tilde{i}+r}} - 1 \rangle = Z^{-1} q^N \sum_{\tilde{D} \subset \mathcal{L}_D} (u^*)^{b(\tilde{D})} q^{n(\tilde{D})} \quad (4.21)$$

where $u = e^{K^*} - 1$; $K^*(K)$ being given by Eq. (10) of the Appendix. The graphs \tilde{D} on the dual lattice \mathcal{L}_D now contain all possible graphs which have a seam of missing links between the plaquettes dual to \tilde{i} and $\tilde{i} + r$ (the seam being dual to the path connecting \tilde{i} , $\tilde{i} + r$ in \tilde{G}).

The extension of the above considerations to the 3d Ising model is also given in Savit (1980). One finds, upon performing a duality transformation on the correlation function $\langle \sigma_{\tilde{i}} \sigma_{\tilde{i}+r} \rangle$ that

$$\langle \sigma_{\tilde{i}} \sigma_{\tilde{i}+r} \rangle \xrightarrow{\text{Duality}} \begin{array}{l} \text{Partition function of the} \\ \text{gauge coupling theory where} \\ \text{for all the plaquettes pierced} \\ \text{by a path connecting } \tilde{i}, \tilde{i} + r, \\ K_p \rightarrow -K_p : \\ \hline \text{Partition function of the frus-} \\ \text{tration free gauge theory.} \end{array} \quad (4.22)$$

with the disorder variables again acting as sources and sinks of a line of defects, this time in the dual gauge system.

The correlation functions (4.18) and (4.22) are clearly independent of the position of the paths Γ apart from their

be in the direction 1. The coupling constants have been normalized by a constant factor $q / (q - 1)$.

Replacing an unfrustrated plaquette by a frustrated one now involves the replacement

$$K_p \rightarrow -K_p / (q - 1) .$$

at that plaquette (Eq. 3.11). Taking the limit $K_p \rightarrow \infty$, one sees that at the site dual to this plaquette

$$h \rightarrow \ln (q - 1) - i \pi ,$$

giving a factor, in the partition function, that is precisely

$$\exp \{ [\ln (q - 1) - i \pi] \delta_{\sigma_{\bar{i}}, 1} \} = 1 - q \delta_{\sigma_{\bar{i}}, 1} .$$

At the sites dual to the unfrustrated plaquettes ($K_p > 0$), $\lim_{K_p \rightarrow \infty} h(K_p) = 0$. Once more, we have

$$\begin{aligned} & \lim_{K_p \rightarrow \infty} Z \{ \phi_p \}_{K, K_p} / Z \{ \phi_p = 1 \}_{K, K_p} \quad (4.15) \\ & = \lim_{K_p \rightarrow \infty} \langle \prod_{\bar{i}} (q \delta_{\sigma_{\bar{i}}, 1} - 1) \rangle_{K^*(K)} \exp n K_p (2 - q) / (q - 1) \end{aligned}$$

where the product runs over the sites dual to the frustrated plaquettes and n is the number of frustrations. Note that the RHS of Eq. (4.15) is in the usual form of an n -point correlation function for the Potts model, in the absence of a field, at the uniform coupling given by $K^*(K)$.

Disorder Variables

Let us take a step back and consider how the dual variables are related to the original ones. To do this, it is instructive to go back to Eq. (4.1) and rewrite it in terms of spin variables. Let us set the plaquette coupling to zero. Then, from Eqs. (4.1) and (4.8),

$$\begin{aligned} Z &= \sum_{\{s_i\}} \exp [K \sum_{(ij)} s_i s_j] \\ &= 2^{N-1} (\cosh K)^E \sum_{\{\sigma_i\}} \exp [K^* \sum_{\bar{i}\bar{j}} (\sigma_{\bar{i}} \sigma_{\bar{j}} - 1)] \quad (4.16) \end{aligned}$$

where we have denoted the dual spin variables by $\sigma_{\tilde{i}}$. Not that there is no one to one correspondance between the configurations of the s and the σ (Savit 1980). However, the relationship (4.9) maps the high temperature region of one model into the low temperature region of its dual. If there is a phase transition to an ordered phase, the critical temperature for this self dual model is uniquely given by

$$K_c = -1/2 \ln \tanh K_c \tag{4.17}$$

Moreover, for $K > K_c$ ($K^* < K_c$) the order parameter $\langle s \rangle \neq 0$ ($\langle \sigma \rangle = 0$) and vice versa. Thus in the temperature region that s is disordered, σ is ordered, and vice-versa. With K^* as a function of K (Eq. 4.9) we can call $\langle \sigma \rangle_{K^*(K)}$ a *disorder parameter*. (Kadanoff and Ceva 1971, Fradkin et al. 1978, Savit 1980). The usefulness of this term will be more apparent when we consider the *disorder-disorder correlation function*, which is nothing but the correlation function of the dual variables at an inverse temperature $K^*(K)$.

$$\langle \sigma_{\tilde{i}} \sigma_{\tilde{i}+r} \rangle = \sum_{\{\sigma_{\tilde{i}}\}} \exp [K^* \sum_{\tilde{i}\tilde{j}} (\sigma_{\tilde{i}} \sigma_{\tilde{j}} - 1)] \prod_{\Gamma_{\tilde{i},\tilde{i}+r}} \sigma_{\tilde{k}} \sigma_{\tilde{l}} / Z(K^*) \tag{4.18}$$

where $\Gamma_{\tilde{i},\tilde{i}+r}$ is any path connecting the points \tilde{i} , $\tilde{i}+r$ and (\tilde{k}, \tilde{l}) are links that lie on $\Gamma_{\tilde{i},\tilde{i}+r}$. (This particular cancellation, due to the fact that $(\sigma_{\tilde{i}})^2 = 1$ is of course peculiar to the Ising model.) Now we can again use the identity (4.12): notice that replacing K^* by $K^* - i\pi/2$ in Eq. (4.16) for those links lying on $\Gamma_{\tilde{i},\tilde{i}+r}$, will give precisely the numerator in Eq. (4.18). Now making the duality transformation on the RHS of Eq. (4.18) we find (with the cancellation in the numerator and denominator of spin independent terms)

$$\langle \sigma_{\tilde{i}} \sigma_{\tilde{i}+r} \rangle = \sum_{\{s_i\}} \exp [\sum K_{ij} s_i s_j] / Z(K(K^*)) \tag{4.19}$$

where $K_{ij} = K(K^*)$ on all links except those dual to the path $\Gamma_{\tilde{i},\tilde{i}+r}$ where $K_{ij} = -K(K^*)$ (Kadanoff and Ceva 1971, Savit 1980). The situation is illustrated in Fig. 7. Observe that the insertion of negative couplings on those bonds intersecting the

The above calculation can be generalized, among, to Z_N models (Savit 1980; here they are called vector Potts models) where the Hamiltonian has the form

$$H_p = \sum_{(ij)} \cos 2\pi p (s_i - s_j + r_{ij}) / N \quad (4.10)$$

where the s_i are now angle variables, taking on values $2\pi q / N$, $q = 0, \dots, N-1$; and to models with continuous symmetry, e.g., the x-y model (Savit 1980). However, the Z_N models are not self-dual, although the dual model also has Z_N symmetry (Savit 1980). Note, however, that our vector Potts model can be written as a sum of such models, in fact

$$H_{\text{vector Potts}} = \sum_{p=0}^{N-1} H_p$$

and it is also self-dual. The derivation of the duality relation proceeds very much like the standard Potts model (Wu 1982). I give a derivation of the duality relation in the gauge representation of the partition function, in the Appendix. Note that duality is a local transformation, so that non-uniform interactions, as in (4.10) can be easily accommodated.

Partition function of system with frustrations

Now let us return to Eq. (4.1). Recall from Eq. (3.19) that we could represent the partition function of a pure spin system with quenched — in frustrations by inserting in the gauge coupling term in Eq. (4.1) a set of numbers ϕ_p , such that $\phi_p > 0$ if the plaquette is unfrustrated and $\phi_p < 0$ if it is frustrated, and then taking the limit $K_p \rightarrow \infty$. In the present case, this would amount to nothing more than replacing K_p by $-K_p$ at those plaquettes where there is a frustration before taking the limit $K_p \rightarrow \infty$. The effect this has on the dual couplings (Eq. 4.9) is that the field at the sites dual to those plaquettes would be replaced by

$$h \rightarrow h - i\pi / 2 \quad (4.11)$$

Inserting this in Eq. (4.8), and using the identity

$$\exp [i\pi (1-s) / 2] = s \quad (4.12)$$

for $s = \pm 1$ we see that (for finite K_p)

$$Z \{ \phi_p \} / Z \{ \phi_p \equiv 1 \} = \langle \prod_{\tilde{i}'} s_{\tilde{i}'} \rangle_{K^*, h} \quad (4.13)$$

where the \tilde{i}' are sites dual to the frustrated plaquettes (Kadanoff and Ceva 1971, Fradkin et al. 1978). (Note that if we had factored out the constant terms from Eq. (4.8) we would have gotten $\exp(-i\pi s/2) = -is$ giving out a factor of $(-i)^n$, $n =$ number of frustrations, in front of the correlation function in Eq. 4.13). In order to quench the frustrations, we can now take $K_p \rightarrow \infty$ ($h \rightarrow 0$)! Thus the partition function of an Ising model with n frustrations, normalized by the unfrustrated partition function, is equal to an n -point correlation function of the dual system (Fradkin et al. 1978).

Expression (4.13) also gives an immediate way of writing down the difference in free energies between a system with two frustrations and an unfrustrated system. Obviously

$$\begin{aligned} -\beta \Delta F &= \ln Z \{ \phi_p \} - \ln Z \{ \phi_p \equiv 1 \} \\ &= \ln \langle \prod_{\tilde{i}'} s_{\tilde{i}'} \rangle_{K^*, \lim h \rightarrow 0} \end{aligned} \quad (4.14)$$

and this gives us a way of defining an *effective interaction* between frustrations (Fradkin et al. 1978, Savit 1980) with the excess free energy due to two frustrations in an unfrustrated background, as a function of r , the separation of the frustrations, going asymptotically as r (diverging) for $K^* < K_c$, and decaying exponentially with r for $K^* > K_c$.

The generalization to the Potts case is straightforward. One obtains the duality relations (see Appendix)

$$\begin{aligned} K^* &= -\ln [(e^K - 1) / (e^K + q - 1)] \\ h &= -\ln [(e^{Kp} - 1) / (e^{Kp} + q - 1)] \end{aligned}$$

where h is a field acting on the sites \tilde{i}' of the dual lattice, via a coupling of the form $h \delta_{\sigma_{\tilde{i}', 1}}$. Here the Potts spins are represented via the scalar variables $\sigma_{\tilde{i}'}$, which take on values between 1 and q , and the field has been chosen (arbitrarily) to

THE LX RAY SPECTRUM OF ARGON, KRIPTON AND XENON (*)

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ABSTRACT — The LX-Ray spectrum of argon, krypton and xenon is interpreted in terms of the initial distribution of single and multiple vacancies. The relative intensity values of the diagram lines (I_d), hidden satellites (I_h) and visible satellites (I_v) is calculated.

The LX-Ray satellites are due to the following processes in multihole configurations:

1. Satellites originated by LM and LN double holes, created by Coster-Kronig (C. K.) $L_3 \rightarrow L_{1,2}$ and $L_2 \rightarrow L_1$ transitions or due to shake-off (s.o.) M, N following the L_i ($i = 1, 2, 3$) ionization. The satellites due to double ionized states can be divided in several classes: $LN \rightarrow MN$; $LN \rightarrow NN$; $LM \rightarrow MM$; $LM \rightarrow MN$.

The $LN \rightarrow MN$ and $LN \rightarrow NN$ satellites are not separated from the parent lines (hidden satellites).

2. Satellites due to shake-off and Coster-Kronig transitions which produce states L_iMM , L_iMN and L_iNN ; the last one leads to hidden satellites.

We can generalize the following conclusions: satellites which arise from LM and LMX states are separated from the parent lines; satellites due to LN or LNN states coincide with parent lines.

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The number of diagram photons from single-hole states in the L_i subshells is given by

$$F_i(L_i) = n_i(L_i) \cdot P_{L_i}^R / (P_{L_i}^R + P_{L_i}^A) \quad (i = 1, 2, 3) \quad (1)$$

For a $L_i \rightarrow X$ transition the number of diagram photons is

$$F_i(L_i) \cdot P_{L_i X}^R / P_{L_i}^R \quad (i = 1, 2, 3) \quad (2)$$

We denote by $n_i(L_i)$ the vacancies in the L_i level following the initial ionization and the rearrangement by Coster-Kronig transitions and shake-off processes; $P_{L_i}^R$ and $P_{L_i}^A$ correspond respectively to the radiative and Auger probabilities in atoms single ionized in the L_i level.

The relations (1) and (2) are valid for double and triple ionized states; however the parameters involved are respectively n'_{L_i} , $P_{L_i}^R$, $P_{L_i}^A$, $P_{L_i Y, XY}^R$ and n''_{L_i} , $P_{L_i}^R$, $P_{L_i}^A$, $P_{L_i YZ, XYZ}^R$.

In the present work we assume $P = P' = P''$. The intensity ratios of visible satellites to diagram lines I_v / I_d and hidden satellites to diagram lines I_h / I_d are respectively

$$I_v / I_d = [n'_i(L_i M) + n''_i(L_i MM) + n''_i(L_i MN)] / n_i(L_i)$$

and

$$I_h / I_d = [n'_i(L_i N) + n''_i(L_i NN)] / n_i(L_i)$$

The triple ionizations are due to shake-off and Coster-Kronig processes or double Coster-Kronig transitions; obviously $L_1 XY = 0$.

These ratios for the elements argon, kripton and xenon have been calculated in the present work; the values for L_1 , L_2 and L_3 levels are displayed in tables 1, 2 and 3.

TABLE 1 — Ratios of satellite to diagram lines (L_1 level).

| Z | I_h (s.o.) / I_d | I_v (s.o.) / I_d |
|----|----------------------|----------------------|
| 18 | 0 | 0.167 |
| 36 | 0.161 | 0.058 |
| 54 | 0.214 | 0.007 |

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NOTE ADDED IN PROOF: The representation chosen for the frustration function of the q-state vector Potts model in this paper leads to an asymmetry in the plaquette couplings (viz. Eqs. (3.19, 3.20), and therefore to vanishing weights for the frustrated configurations for $q \neq 2$. This may be remedied by choosing a slightly different representation. Details are given in a forthcoming publication.

where the graphs

G consist of bonds and lattice points on the lattice \mathcal{L} .

G_p consist of plaquettes on \mathcal{L} .

Performing the sums over the spin and gauge variables, yields, after a bit of work,

$$\exp(NK_p/q) \cdot Z \{ \phi_p = 1 \}_{K_p} = q^{E+N} \sum_{G, G_p} \sum_{C \subset \mathcal{L}} (u/q)^{b(G)} (v/q)^{p(G_p)} q^{c_1(G, G_p)} \quad (6)$$

where E and N are the number of edges and vertices in \mathcal{L} , $b(G)$ is the number of bonds in G , $p(G_p)$ is the total number of plaquettes in G_p , and $c_1(G, G_p)$ is the number closed circuits in G that are completely filled by clusters of plaquettes in G_p .

Now consider the (unfrustrated) random vector Potts model in the presence of a field. The partition function is

$$Z(K^*, h) = \sum_{\{s\}} \exp \left[K^* \sum_{(\tilde{i}\tilde{j})} s_{\tilde{i}}^\dagger \psi_{\tilde{i}\tilde{j}} s_{\tilde{j}} + h \sum_{\tilde{i}} s_{\tilde{i}}^\dagger s_0 \right] \quad (7)$$

where s_0 has been chosen in the 1 (Potts) direction. (The interaction $h s_{\tilde{i}}^\dagger s_0$ may be written $h \delta_{\sigma_{\tilde{i}}, 1}$ in terms of the scalar variables $\sigma_{\tilde{i}}$). The Whitney polynomial representation is

$$Z(K^*, h) = \sum_{\{s\}} \sum_{G, G_k} \sum_{\tilde{k}} \prod_{(\tilde{i}\tilde{j}) \in \tilde{G}} u^* s_{\tilde{i}}^\dagger \psi_{\tilde{i}\tilde{j}} s_{\tilde{j}} \prod_{K \in G_k} w s_k^\dagger s_0 \quad (8)$$

where $u^* = e^{K^*} - 1$, $w = e^h - 1$, and the graphs

\tilde{G} consist of vertices (points) and bonds on the dual lattice $\tilde{\mathcal{L}}$

G_k consist only of points.

Performing the summation over the spin variables gives,

$$Z(K^*, h) = \sum_{\tilde{G}, G_k} (u^*)^{b(\tilde{G})} w^{p(G_k)} q^{m(\tilde{G}, G_k)} \quad (9)$$

where b has the same meaning as before, $p(G_k)$ is the total number of points in G_k , and $m(\tilde{G}, G_k)$ is the number of connected graphs in \tilde{G} that do not contain any points of G_k .

Define, as usual, the dual of the graph G (on \mathcal{L}) to be the graph obtained on $\tilde{\mathcal{L}}$ by placing bonds (rotated by 90°) on all links on \mathcal{L} not occupied by bonds in G . Define the dual of G_p to be the graph obtained by placing points on all plaquettes in \mathcal{L} not occupied by plaquettes in G_p . Clearly, the graphs generated are of the type \tilde{G} and G_k . Moreover, observe that

$$\begin{aligned} b(G) &= E - b(\tilde{G}) \\ p(G_p) &= N - p(G_k) \\ c_1(G, G_p) &= m(\tilde{G}, G_k) \end{aligned}$$

if G is taken to be the dual of G and G_k the dual of G_p . Re-expressing Eq. (6) in terms of the sums over G and G_k , we have

$$e^{NK_p/q} Z \{ \phi_p = 1 \}_{K_p} = u^E v^N Z(K^*, h)$$

provided that

$$\begin{aligned} (u^*)^{-1} &= u/q \\ (w)^{-1} &= v/q \end{aligned}$$

yielding the duality relations

$$\begin{aligned} K^* &= -\ln [(e^K - 1) / (e^K + q - 1)] \\ h &= -\ln [(e^{K_p} - 1) / (e^{K_p} + q - 1)] . \end{aligned} \tag{10}$$

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Then, for only two frustrations in $\{\phi_p\}$, this probability behaves with the distance between the frustrations according to the exactly known two-point correlation function of the (field free) Ising model in two dimensions (Schuster 1979). Recall that K_f is given as a function of the concentration x of (in this case) FM bonds (Eq. 3.27). Thus, Eqs. (4.26) and (4.13) predict a phase transition in the system of frustrations. With $K_f = -1/2 \ln(2x - 1)$ we have:

i) $1 > x > x_0 = K_f^*_{crit}$ ($\sim .7072$). The probability to find two frustrations separated by r decays like $\exp(-r/\xi)$ with ξ being the correlation length of the Ising model at temperature K_f^* .

ii) $x = x_0$. ξ diverges, so that one obtains 'pair dissociation' of frustrations.

iii) $x < x_0$. In this case there is a finite probability to find a single frustrated plaquette — thus necessarily an infinite 'ladder' of AFM bonds in the system (see Fig. 1c) (Schuster 1979).

Notice that FM order is already destroyed at $x < x^* = .91$ (Vannimenus and Toulouse 1977) by the possibility of having infinite strings of frustrated plaquettes — at x_0 , however, new types of 'domain walls' (defects of infinite length on the spin system) associated with the 'ladders' of AFM bonds appear. Thus the ground state seems to be qualitatively changed as we go through x_0 . Although there is no finite temperature phase transition for this system, i.e., it remains paramagnetic down to $T = 0$, the singularities introduced into the quenched average for the free energy, via the probabilities $P\{\phi_p\}$ persist at all temperatures! This was essentially foreseen by Schuster (1979), and it also has its generalization to the arbitrary- q Potts model.

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APPENDIX

Here I present the duality transformation for the Potts model in the presence of quenched randomness. (A different treatment has been given by Jauslin and Swendsen (1981).)

Consider the partition function

$$Z \{ \phi_p \} = \lim_{K'_p \rightarrow \infty} \sum_{\{ \psi_{ij} \}} \sum_{\{ s_i \}} \exp (K \sum_{(ij)} s_i^\dagger \psi_{ij} s_j) \cdot \exp [K'_p \sum_p \phi_p (\text{Tr} \prod_p \psi - 1) / (q - 1)] \quad (1)$$

A slightly more condensed notation has been used that in Section 3, which should be self explanatory. The bond labels have been dropped from the gauge variables appearing in products around plaquettes, as in $\prod_p \psi$. The frustration function ϕ_p is defined via Eq. (3.11). Extracting a constant factor from the sum, and defining

$$K_p = q K'_p / (q - 1) ,$$

we have

$$Z \{ \phi_p \} = \lim_{K_p \rightarrow \infty} \exp (-NK_p / q) \sum_{\{ \psi \}} \sum_{\{ s \}} \exp (K \sum_{ij} s_i^\dagger \psi_{ij} s_j) \cdot \exp [K_p \sum_p (\text{Tr} \prod_p \psi) / q] \quad (2)$$

Define

$$\begin{aligned} u &= e^K - 1 \\ v &= e^{K_p} - 1 . \end{aligned} \quad (3)$$

Then

$$\begin{aligned} \exp (K s_i^\dagger \psi_{ij} s_j) &= (s_i^\dagger \psi_{ij} s_j) u + 1 \\ \exp (K_p \text{Tr} \prod_p \psi / q) &= (\text{Tr} \prod_p \psi) v / q + 1 . \end{aligned} \quad (4)$$

Now setting all $\phi_p = 1$, and going over to the Whitney polynomial representation, we have for finite K_p ,

$$Z \{ \phi_p = 1 \}_{K_p} = \exp (-NK_p / q) \cdot \sum_{\{ \psi \}} \sum_{\{ s \}} \sum_{G, G_p \subset \mathcal{E}} \prod_{(ij) \in G} u s_i^\dagger \psi_{ij} s_j \prod_{p \in G_p} (\text{Tr} \prod_p \psi) v / q \quad (5)$$

TABLE 2 — Ratios of satellite to diagram lines (L_2 level).

| Z | $I_h(\text{C.K.})/I_d$ | $I_h(\text{s.o.})/I_d$ | $I_h(\text{s.o.} + \text{C.K.})/I_d$ | $(I)_{ht}/I_d$ | $I_v(\text{C.K.})/I_d$ | $I_v(\text{s.o.})/I_d$ | $I_v(\text{s.o.} + \text{C.K.})/I_d$ | $(I)_{vt}/I_d$ |
|----|------------------------|------------------------|--------------------------------------|----------------|------------------------|------------------------|--------------------------------------|----------------|
| 18 | 0 | 0 | 0 | 0 | 0.240 | 0.178 | 0.040 | 0.458 |
| 36 | 0.029 | 0.164 | 0.005 | 0.198 | 0.213 | 0.051 | 0.054 | 0.318 |
| 54 | 0.179 | 0.219 | 0.045 | 0.443 | 0 | 0.008 | 0.001 | 0.009 |

TABLE 3 — Ratios of satellite to diagram lines (L_3 level).

| Z | $I_h(\text{C.K.})/I_d$ | $I_h(\text{s.o.})/I_d$ | $I_h(\text{s.o.} + \text{C.K.})/I_d$ | $(I)_{ht}/I_d$ | $I_v(\text{C.K.})/I_d$ | $I_v(\text{s.o.})/I_d$ | $I_v(\text{s.o.} + \text{C.K.})/I_d$ | $(I)_{vt}/I_d$ |
|----|------------------------|------------------------|--------------------------------------|----------------|------------------------|------------------------|--------------------------------------|----------------|
| 18 | 0 | 0 | 0 | 0 | 0.240 | 0.177 | 0.040 | 0.457 |
| 36 | 0.062 | 0.163 | 0.015 | 0.240 | 0.224 | 0.051 | 0.050 | 0.325 |
| 54 | 0.208 | 0.217 | 0.042 | 0.467 | 0 | 0.007 | 0.0014 | 0.008 |

The energies of diagram and satellite lines are very close; so the energy corrections can be disregarded. The $n_i(L_i)$, $n'_i(L_i)$ and $n''_i(L_i)$ results have been obtained from ref. [1]; values of shake-off probabilities are from ref. [2] and Coster-Kronig parameters are from ref. [3, 4].

We can conclude that it seems impossible to observe a pure line (true diagram line); the diagram lines so observed are always contaminated by hidden satellites.

Table 1 shows that satellite lines due to L_1 ionization are not negligible as it should be if they were only due to Coster-Kronig transitions.

From tables 2 and 3 we can see that the total values of the ratio $(I_h)_t / I_d$ increase with the atomic number; thus for high values of Z there is a strong contamination of the diagram lines due to hidden satellites.

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